UNCLAS[...] AD-A249 265 [...]COPY - FOR REPRODUCTION PURPOSES (2)

SECURITY C[...]

[...]OCUMENTATION PAGE

DTIC

1a. REPORT [...] Unclassified	1b. RESTRICTIVE MARKINGS
2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution unlimited.
2b. DECLASSIFICATION / DOWNGRADING SCHEDULE	
4. PERFORMING ORGANIZATION REPORT NUMBER(S) FSU Department of Statistics Technical Report No. M-864	5. MONITORING ORGANIZATION REPORT NUMBER(S) ARO 27868.14-MA
6a. NAME OF PERFORMING ORGANIZATION Florida State University — 6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION U. S. Army Research Office
6c. ADDRESS (City, State, and ZIP Code) Department of Statistics B-167 Florida State University Tallahssee, FL 32306-3033	7b. ADDRESS (City, State, and ZIP Code) P. O. Box 12211 Research Triangle Park, NC 27709-2211
8a. NAME OF FUNDING/SPONSORING ORGANIZATION U. S. Army Research Office — 8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER DAAL03-90-G-0103
8c. ADDRESS (City, State, and ZIP Code) P. O. Box 12211 Research Triangle Park, NC 27709-2211	10. SOURCE OF FUNDING NUMBERS PROGRAM ELEMENT NO. / PROJECT NO. / TASK NO. / WORK UNIT ACCESSION NO.

11. TITLE (Include Security Classification)
Markov Chain Simulations of Binary Matrices

12. PERSONAL AUTHOR(S)
William B. Krebs

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
Technical	FROM ____ TO ____	January 1992	18

16. SUPPLEMENTARY NOTATION
The view, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy, or decision, unless so designated by other documentation.

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	Markov chain, spectral estimate, binary matrices rapid mixing.

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

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92-11247

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT ☐ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT. ☐ DTIC USERS	21. ABSTRACT SECURITY CLASSIFICATION Unclassified
22a. NAME OF RESPONSIBLE INDIVIDUAL	22b. TELEPHONE (Include Area Code) — 22c. OFFICE SYMBOL

DD FORM 1473, 84 MAR — 83 APR edition may be used until exhausted. All other editions are obsolete.

SECURITY CLASSIFICATION OF THIS PAGE
UNCLASSIFIED

92 4 27 434

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By

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Florida State University

January 1992

FSU Technical Report No. M–864

USARO Technical Report No. D–124

Key Words: Markov chain, spectral estimate, binary matrices, rapid mixing

AMS 1980 Subject Clasification Nos. 60J20, 68J05, 05C50

Markov Chain Simulations of Binary Matrices

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1. Introduction:

Let M be a given $m \times n$ matrix whose entries are 0s and 1s. We want to choose a matrix N distributed uniformly over those $m \times n$ 0–1 matrices with the same row and column sums as M.

Let $M[i_1, i_2; j_1, j_2]$ be a 2×2 submatrix of M taking one of the two forms

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Exchange 0s and 1s in $M[i_1, i_2; j_1, j_2]$, and call the resulting matrix M'. It is clear that the row and column sums M' are the same as those of M. the operation taking M to M' is called an *interchange*.

The interchange operation defines a graph structure on the binary matrices whose row and column sums equal those of M. The set of such matrices forms our vertex set; if N and N' are vertices, an edge joins them if there is an interchange taking N to N'. Call this graph the *interchange graph*.

One way of simulating an approximately uniformly distributed 0–1 matrix with fixed row and column sums is by defining an irreducible Markov chain $\{M_i\}$ on the interchange graph with uniform stationary distribution. If T is a function defined on 0–1 matrices, then

$$\frac{1}{n}\sum_{1}^{n} T(M_i) \rightarrow ET$$

with probability 1. If M_0 is a fixed matrix in this set, we can then estimate $P[T > T(M_0)]$ by simulating the Markov chain and computing empirical probabilities after a suitably large number of transitions. In particular, let D be the maximum degree of any vertex in the interchange graph, let $p < D^{-1}$, and for a vertex M, define

$$\begin{aligned} P(M, M') &= p \quad \text{if } \{M, M'\} \text{ is an edge} \\ P(M, M) &= 1 - Dp \\ P(M, M') &= 0 \quad \text{otherwise} \end{aligned}$$

It may be shown that these transitions define an irreducible Markov chain on the interchange graph with uniform stationary distribution. Call such a chain a modified random walk.

The effectiveness of this approach depends on how rapidly the distribution of M_i converges to the uniform distribution. For binary matrices with fixed row and column sums, the state space may be very large indeed. In general, it is approximately a hyper-exponential function of the size of the matrix M. See Good and Crook [4] for asymptotic approximations, as well as exact recurrence formulas for certain special cases. Ideally, we want the number of steps needed for the distribution of M_i to converge to be a polynomial in the "size" of M. The main result of this paper is that for a particular modified random walk on the interchange graph, the eigen value defining this "relaxation time" is bounded by a polynomial in the number of non-zero entries and the number of rows and columns in M, but is otherwise independent of the number of 0-1 matrices satisfying the row-column sum restrictions.

Binary matrices with row and columns sums fixed can be regarded as matrix representations of bipartite graphs with a given degree sequence. The problem of simulating general graphs with a fixed degree sequence can be approached by similar methods. Here, one constructs a Markov chain on a space of graphs by selectively adding, removing, or exchanging individual edges in the graph. Again, under certain restrictions on the degree sequence, we show that the subdominant eigenvalue of this chain is bounded by a polynomial in the total number of edges.

Uniform distributions on spaces of integer matrices subject to various row and column constraints arise in a number of areas. A very specific example is in biogeographical ecology. Here we have a collection of habitats under study and a collection of species of interest. For each habitat, we know which species occur in that habitat. If we write the data as an incidence matrix of species in habitats, we get a binary matrix, say M_0.

Ecologists are particularly interested in whether or not two species compete. One way of assessing the degree of competition between two species i and j is to count the number t_{ij} of habitats where both species occur and then compute the probability that a random arrangement of species in habitats would have t_{ij} or fewer common habitats for species i and j. We restrict the random arrangements by requiring that in any such arrangement, each species must occupy the same number of habitats and each habitat must support the same number of species as in our original M_0. Then the desired probability is $P[T_{ij}(M) > t_{ij}]$, where M is uniformly distributed over binary matrices with row and column sums equal to those of M_0. See Simberloff[9], Conner and Simberloff[3], and Simberloff and Zaman [10] for more detailed discussion of this problem.

Another place where random integer matrices arise is in the study of contingency tables. Here, conventional statistical analysis might begin by testing for independence of rows and columns by means of the χ^2 statistic. If the hypothesis of independence is strongly rejected, there is a need for some alternative probability model to describe the table.

One alternative that has been proposed is a uniform distribution on the space of contingency tables with a given set of marginal totals. In the setting of the present paper, the state space may be regarded as the set of contingency tables with the further restriction that all entries be either 0 or 1. Diaconis and Efron [5] discuss this model for contingency tables, along with a family of other models. They provide a formula for computing approximate probabilities for this distribution. Markov chain simulations using the interchange formula provide an alternative means for computing probabilities for this distribution.

In Section 2 of this paper, we review some standard definitions and notation for binary matrices, graph theory, and Markov chains. In Section 3, we prove an essential graph theory lemma, and then apply it to bounding the eigenvalue of a Markov chain for generating an almost uniformly distributed graph with a fixed degree sequence. The main results of this paper are Propositions 6 and 7 in section 4, where we compute a bound for the rate of convergence of a random walk on the interchange graph for a space of binary matrices. Afterwards, we discuss the convergence rates of functions of the chain.

2. Some Definitions:

For integer sequences $\mathbf{r} = (r_1, \ldots, r_m)$ and $\mathbf{s} = (s_1, \ldots, s_n)$, let be $\mathfrak{A}(\mathbf{r}, \mathbf{s})$ be the set of binary matrices with row sums r and column sums $\mathbf{s}$, and suppose that $\mathfrak{A}(\mathbf{r}, \mathbf{s}) \neq \emptyset$.

Define a graph $\mathcal{I} = (\mathfrak{A}, \mathcal{E})$, with $\mathfrak{A} = \mathfrak{A}(\mathbf{r}, \mathbf{s})$, and edge set $\mathcal{E}$ defined by $\{M, M'\} \in \mathcal{E}$ if there exist rows i_1 and i_2 and columns j_1 and j_2 such that

$$\begin{aligned} M[i_1, i_2; j_1, j_2] &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} & \qquad M'[i_1, i_2; j_1, j_2] &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \text{or} \\ M[i_1, i_2; j_1, j_2] &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} & \qquad M'[i_1, i_2; j_1, j_2] &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \end{aligned} \tag{1}$$

and $M[k, l] = M'[k, l]$, for $k \neq i_1, i_2$ or $l \neq j_1, j_2$. Call the operation taking M to M' an *interchange*, and $\mathcal{I}$ the *interchange graph* on $\mathfrak{A}(\mathbf{r}, \mathbf{s})$. We will often write either of these two interchanges in the form $(i_1, i_2; j_1, j_2)$.

One important interpretation of $\mathfrak{A}(\mathbf{r}, \mathbf{s})$ is as the set of bipartite graphs with bipartition $\{1, \ldots, m; m+1, \ldots, m+n\}$ and degree sequence $r_1, \ldots, r_m; s_1, \ldots, s_n$. We shall use either the graph or the matrix interpretation of $\mathfrak{A}$, according to convenience.

For binary matrices $A = [a_{ij}]$ and $B = [b_{ij}]$, let

$$A \oplus B = [a_{ij} + b_{ij} \pmod 2] \qquad A \vee B = [\max\{a_{ij}, b_{ij}\}].$$

For future reference, we will review some standard graph theory notions. Let $G = (V, \mathcal{E})$ be an arbitrary graph. Say that $\gamma = \{x_0, x_1, \ldots, x_k, x_{k+1} = x_0\}$ is a *circuit* if $x_0, \ldots, x_k$ are vertices and $\{x_i, x_{i+1}\}$ is an edge for $i = 0, \ldots, k$. If, in addition, $x_0, \ldots, x_k$ are distinct we say that γ is *elementary*. Say that G is *Eulerian* if there exists a circuit β that traverses every edge in $\mathcal{E}$ exactly once; we call the circuit β

an Eulerian circuit. We recall the elementary result that a graph is Eulerian if and only if it is connected and contains either no or two vertices of odd degree.

The fundamental result on interchanges is that the interchange graph is connected, known as Ryser's Theorem.

Theorem 1. *Let A and B be matrices in $\mathfrak{A}(\mathrm{r},\mathrm{s})$ and let $B-A = C_1+\cdots+C_q$, where $C_1,\ldots,C_q$ are disjoint elementary circuits. Let the number of non-zero entries of C_i be $2k_i$, $i = 1,\ldots,q$. Then there exists a sequence of $k_1+\cdots+k_q-q$ interchanges which transforms A into B.*

Proof: This is Theorem 3.2 in Brualdi[2].

We will also need some standard ideas about Markov chains. Let P be an irreducible aperiodic Markov transition matrix on some finite set. Then it is well-known that P has a unique stationary distribution π, and $\|P^n(x,\circ) - \pi(\circ)\| < \beta_1^n$, where β_1 is the subdominant eigenvalue of P.

Given some knowledge of the geometry of our state space, we can bound β_1. Let P be reversible, so that $\pi(x)P(x,y) = \pi(y)P(y,x)$ for all states x and y. Let $Q(x,y) = \pi(x)P(x,y)$. For each pair $\{x,y\}$ in the state space, suppose there is a path γ_{xy} connecting x to y. Let

$$\eta = \max_e Q(e)^{-1} \sum_{\gamma_{xy} \ni e} \pi(x)\pi(y).$$

Then, the following theorem holds.

Theorem 2. *For a reversible, irreducible Markov chain P, the second largest eigenvalue satisfies*

$$\beta_1 \leq 1 - \frac{1}{8\eta^2}$$

Proof: This is Proposition 7 in Diaconis and Stroock[6].

Finally, for arbitrary matrices A, B, define the matrix

$$\mathrm{diag}(A,B) = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}$$

If $\lambda_1, \ldots, \lambda_n$ are real numbers, diag$(\lambda_1, \ldots, \lambda_n)$ will denote the $n \times n$ diagonal matrix with entries $\lambda_1, \ldots, \lambda_n$.

3. Generating Graphs by Edge Perturbations:

Let $\mathbf{d} = (d_1, \ldots, d_n)$ be a sequence of positive integers. Let $\mathcal{G}(\mathbf{d}) = \mathcal{G}$ be the set of graphs with degree sequence $\mathbf{d}$, and suppose that $\mathcal{G} \neq \emptyset$. Let $\mathcal{G}'$ be the set of graphs with degree sequences $\mathbf{d}' = (d'_1, \ldots, d'_n)$ satisfying

i. $d'_i \leq d_i$, $i = 1, \ldots, n$

ii. $\sum_1^n (d_i - d'_i) = 2$

Let $\mathcal{S} = \mathcal{G} \cup \mathcal{G}'$. In [8], Section 2, Jerrum and Sinclair define the following set of transitions for a Markov chain on $\mathcal{S}$.

i. Select an edge $\{i, j\}$ uniformly at random.

ii. If $G \in \mathcal{G}$ and $\{i, j\}$ is an edge in G, let $H = G - \{i, j\}$.

iii. If $G \in \mathcal{G}'$, $\{i, j\}$ is not an edge in G, and the degree of i is less than d_i, let $H = G + \{i, j\}$. If the degree of j exceeds d_j select an edge $\{j, k\}$ uniformly at random and delete it.

iv. In all other cases, do nothing.

Let $d_{max} = \max(d_1, \ldots, d_n)$, and let $N = \frac{1}{2} \sum_1^n d_i$ be the number of edges in G. Say that $\mathbf{d}$ s *p-stable* if $N > d_{max}^2 - d_{max}$. In [8], Jerrum and Sinclair remark without proof that a Markov transition matrix defined by *i. – iv.* will have a subdominant eigenvalue that is bounded by a polynomial in $(d_1, \ldots, d_n)$ if $\mathbf{d}$ is p-stable. We now show this explicitly.

Proposition 3. *The subdominant eigenvalue of the transition matrix induced by i.–iv. satisfies the bound*

$$\beta_1 \leq 1 - \frac{1}{8} \left(N^4 d_{max}\right)^{-2}$$

Proof: Our approach follows that of Jerrum and Sinclair [7], [8]. As in these papers, we will define a system of canonical paths in $\mathcal{S}$, use these to bound η and then estimate the subdominant eigenvalue of the transition matrix. As a first step we prove a graph theory lemma.

Lemma 4. *Let $G = (V, \mathcal{E})$ be a connected graph. Suppose $\mathcal{E} = \mathcal{E}_1 \cup \mathcal{E}_2$, $\mathcal{E}_1 \cap$*

$\mathcal{E}_2 = \emptyset$, *and that* $|e_1(v)| = |e_2(v)|$ *for all* $v \in V$, *where* $e_1(v)$ *and* $e_2(v)$ *are the edges in* $\mathcal{E}_1$ *and* $\mathcal{E}_2$, *respectively, incident to* v. *Then* G *has an Eulerian circuit* $\{v_0, v_1, \ldots, v_{2n-1}, v_0\}$ *such that* $\{v_{2i}, v_{2i+1}\} \in \mathcal{E}_1$ *and* $\{v_{2i+1}, v_{2i+2}\} \in \mathcal{E}_2$ *for* $i = 0, \ldots, n-1$.

Proof: It is easy to see that $|\mathcal{E}|$ is even, say $|\mathcal{E}| = 2n$. The proof follows by an induction on n. The smallest n for which the conditions of the lemma can be satisfied is $n = 2$. For $n = 2$, we have $V = \{1,2,3,4\}$, $\mathcal{E}_1 = \{\{1,2\},\{3,4\}\}$ and $\mathcal{E}_2 = \{\{2,3\},\{4,1\}\}$, within isomorphism. $\gamma = \{1,2,3,4,1\}$ is then the desired circuit.

Now suppose the lemma holds for $n = k$, and let $n = k+1$, so $|\mathcal{E}| = 2k+2$. Choose a vertex v_0 and edges $\{v_0, v_1\}$ and $\{v_1, v_2\}$ in $\mathcal{E}_1$ and $\mathcal{E}_2$, respectively. These exist, by hypothesis. Continuing in the same manner, select vertices $v_3, \ldots, v_{2m}$ so that $\{v_{2i}, v_{2i+1}\} \in \mathcal{E}_1$, $\{v_{2i+1}, v_{2i+2}\} \in \mathcal{E}_2$, for $i = 1, \ldots, m-1$ and all edges are distinct, until you reach the first vertex v_{2m} where such a choice cannot be made. I claim $v_{2m} = v_0$, for if $\{v_{2m}, w\}$ appears in the circuit for all w adjacent to v_{2m}, then an odd number of edges adjacent to v_{2m} must have been crossed prior to stage $2m$. The only vertex in the graph satisfying this requirement is v_0.

Let $\gamma = \{v_0, v_1, \ldots, v_{2m-1}, v_{2m}\}$. If $m = k+1$, then γ is the desired circuit, and we are finished. So, suppose $m < k+1$. Let $\mathcal{F} = \{\{v_{i-1}, v_i\}, i = 1, \ldots, 2m\}$, let $\mathcal{E}' = \mathcal{E} \setminus \mathcal{F}$ and let G' be the subgraph induced by $\mathcal{E}'$. Write $G' = G_1 \cup \cdots \cup G_\nu$ as the union of connected components. Then it is easy to see that each component G_i satisfies the hypotheses of this lemma, with fewer than $2k$ edges. Thus, suitable circuits can be constructed on each G_i and adjoined to γ. The lemma follows. ■

Corollary 5. *Let* $G = (V, \mathcal{E})$ *be a connected graph as in Lemma 4. Suppose there exist vertices* $v_+, v_- \in V$ *such that* $|e_1(v_+)| = |e_2(v_+)| + 1$ *and* $|e_1(v_-)| = |e_2(v_-)| - 1$; *for all other vertices, suppose* $e_1(v) = e_2(v)$. *Then,* G *has an Eulerian path* $\{v_0, v_1, \ldots, v_n\}$ *such that* $v_0 = v_+$, $v_n = v_-$, *and* $\{v_{2i}, v_{2i+1}\} \in \mathcal{E}_1$, $\{v_{2i+1}, v_{2i+2}\} \in \mathcal{E}_2$ *for* $i = 0, \ldots, n-1$.

We now proceed to construct our set Γ of canonical paths. Let $G, H \in \mathcal{G}$ and let $D = G \oplus H$ be the symmetric difference of G and H. Write $D = D_1 \cup \cdots \cup D_k$

where $D_1, \ldots, D_k$ are the connected components of D. Any vertex v in D has the property that the numbers of edges in $G \setminus H$ and $H \setminus G$ incident to v are the same. Thus Lemma 4 applies to each component D_i.

Order the Eulerian subgraphs of $G \cup H$ in some fashion, and for each such Eulerian subgraph, suppose a starting vertex v_0 has been identified. Suppose that $D_1, \ldots, D_k$ is an increasing sequence in the order.

The canonical path from G to H will be defined by *unwinding* $D_1, \ldots, D_k$ in order. The unwinding will be carried out as follows:

i. For each component D_i, fix a starting vertex v. Let $\mathcal{D}_i$ be an ordering of the Eulerian circuits on D_i, with v as starting (and ending) vertex. Note that every Eulerian circuit induces an ordering on the edges of E_i.

ii. Let $\mathfrak{B}_i$ be the set of Eulerian circuits on D_i such that edges in $G \setminus H$ have odd parity and edges in $H \setminus G$ have even parity. (That is, if $\gamma = \{v_0, \ldots, v_{2m}\}$, then $\{v_{2i}, v_{2i+1}\} \in G \setminus H$ and $\{v_{2i+1}, v_{2i+2}\} \in H \setminus G$ for i from 0 to $m-1$.) By Lemma 4, $\mathfrak{B}_i$ is not empty. Let β be the first element in $\mathfrak{B}_i$, with respect to our ordering of $\mathcal{D}_i$.

iii. Suppose $\beta = \{v_0, \ldots, v_{2m}\}$. The unwinding begins by removing $\{v_0, v_1\}$. The next $m-1$ steps consist of adding $\{v_{2i-1}, v_{2i}\}$ and removing $\{v_{2i}, v_{2i+1}\}$ in sequence for $i = 1, \ldots, m-1$. The final step is to add the edge $\{v_{2m-1}, v_{2m}\}$.

Let $\{M, M'\}$ be a transition in the canonical path from G to H, and let v be a vertex in $M \cap M'$. By the definition of canonical paths, $e_G(v) \cap e_H(v) \subset e_{M \cap M'}(v) \subset e_G(v) \cup e_H(v)$. Let $S = M \cup M' \oplus (G \oplus H)$. By elementary set theory,

$$\begin{aligned}
|e_S(v)| &= |e_{M\cup M'}(v) \oplus (e_G(v) \oplus e_H(v))| \\
&= |e_{M\cup M'}(v) \cup (e_G(v) \oplus e_H(v))| - |e_{M\cup M'}(v) \cap (e_G(v) \oplus e_H(v))| \\
&= |e_G(v) \cup e_H(v)| - (|e_{M\cup M'}(v)| - |e_G(v) \cap e_H(v)|) \\
&= |e_G(v)| + |e_H(v)| - |e_{M\cup M'}(v)|
\end{aligned}$$

There are three possible cases to consider. Let i be the unique vertex of degree 2 in $M \oplus M'$. Then $|e_{M\cap M'}(v)| = d_i + 1$, and as $G, H \in \mathcal{G}$, $|e_S(i))| = d_i - 1$. Alternatively, let j be the starting vertex in the cycle γ we are unwinding. Then $|e_M(j)| = |e_{M'}(j)| = d_j - 1$, so $|e_S(j))| = d_j + 1$. For all other vertices k, $|e_G(v)| = |e_H(v)| = |e_{M\cap M'}(v)| = d_k$, so $|e_S(v))| = d_k$.

Define a function $\sigma_\tau(G, H)$ encoding G and H by setting

$$\sigma_\tau(G,H) = \begin{cases} (G \oplus H) \oplus (M \cup M') & \text{if } \tau \text{ begins or ends a circuit} \\ (G \oplus H) \oplus (M \cup M') - e_{G,t} & \text{otherwise} \end{cases}$$

Here, $e_{G,t}$ is the first edge in β.

From the discussion in the last paragraph, it follows that $\sigma_\tau(G, H) \in \mathcal{S}$. Furthermore, σ is one–to–one, since we can reconstruct G and H from $\sigma_\tau(G, H)$ and $M \cup M'$. To see this, let $K = \sigma_\tau(G,H) \oplus (M \cup M')$. If $\sigma_\tau(G, H) \in \mathcal{G}$, then $K = D_1 \cup \cdots \cup D_k$. If $\sigma_\tau(G, H) \in \mathcal{G}'$, then $K = D_1 \cup \cdots \cup D_{i-1} \cup \tilde{D}_i \cup D_{i+1} \cup \cdots \cup D_k$, where $\tilde{D}_i$ has precisely two vertices of odd degree. We recover D_i by adding an edge joining the two odd-degree vertices. D_i is the unique component containing $M \cap M'$, so D_i is the current subgraph in the unwinding.

Let C_i be the set of Eulerian paths on D_i starting at the initial vertex v_i and having the property that edges in $\sigma_\tau(G, H)$ have odd parity prior to $M \oplus M'$ and even parity afterwards. $\beta \in C_i$ so C_i is not empty. Let $\tilde{\beta}$ be the first path in C_i. Then $\tilde{\beta}$ induces a path on D_i such that edges in G and H have odd and even parity respectively. Thus, $\tilde{\beta} = \beta$. G and H can now be identified by unwinding β forwards or backwards from M, as necessary.

To extend canonical paths to the whole of $\mathcal{S}$, we will define a function $G \to \bar{G}$ that will associate a "nearest" member of $\mathcal{G}$ to each element in $\mathcal{S}$. If $G \in \mathcal{G}$, let $\bar{G} = G$. Now, let $G \in \mathcal{G}'$. Following Jerrum and Sinclair[8], define a graph $\bar{G} \in \mathcal{G}$ that is "close" to G. There are two cases to consider.

i. Suppose there are vertices i and j such that $d_i' = d_i - 1$ and $d_j' = d_j - 1$. If $\{i, j\} \notin \mathcal{E}$, let $\bar{G} = G + \{i, j\}$. If $\{i, j\} \notin \mathcal{E}$, then find an edge $\{k, l\}$ such that $\{i, k\}$ and $\{j, l\}$ are not edges and let $\bar{G} = G + \{i, k\} + \{j, l\} - \{k, l\}$. As shown in Jerrum and Sinclair[8], section 3, such an edge always exists, if the sequence d is p-stable.

ii. Alternatively, suppose there is a vertex i such that $d_i' = d_i - 2$. Again, find an edge $\{k, l\}$ such that $\{i, k\}$ and $\{i, l\}$ are not edges and let $\bar{G} = G + \{i, k\} + \{i, l\} - \{k, l\}$.

In either case, since G and $\bar{G}$ differ by at most two edges, at most N^2 graphs G can be associated with any $\bar{G}$.

For $G, H \in S$, define the canonical path from G to H by connecting G to $\bar{G}$, H to $\bar{H}$, and defining the canonical path from $\bar{G}$ to $\bar{H}$ as in the preceding paragraphs. Then, the number of canonical paths crossing any given edge $\{M, M'\}$ is at most $N^4|\mathcal{G}'|$. As before, let $\eta = \max_e Q(e)^{-1} \sum_{\gamma_{xy} \ni e} \pi(x)\pi(y)$. Then,

$$\eta = Q(e)^{-1} \max_e \sum_{\gamma_{xy} \ni e} \frac{1}{|S|^2} \leq 2N|S| \times N^4|S| \times \frac{1}{|S|^2} = 2N^5$$

Apply Theorem 2 to get

$$\beta_1 \leq 1 - \frac{1}{32} N^{-10}$$

This completes the proof of the proposition. ■

Remark: In [8], Jerrum and Sinclair describe an alternative algorithm for almost generating uniform random graphs in $\mathcal{G}(\mathbf{d})$ by tranlating the problem into one of simulating random perfect matchings. Additional structure provided by the matching problem gives the bound

$$\beta_1 \leq 1 - \left(\frac{1}{16n^4(n/2 + 2N)(n-1)} \left(\frac{|\mathcal{G}|}{|\mathcal{G}'|} \right)^2 \right)^2$$

for an arbitrary family $\mathcal{G}(\mathbf{d})$. The p-stability condition gives a sufficient condition for $|\mathcal{G}'|/|\mathcal{G}|$ to be polynomially bounded. If $\mathbf{d}$ is p-stable, then

$$\beta_1 \leq 1 - \left(\frac{1}{16N^4 n^4(n/2 + 2N)(n-1)} \right)^2$$

4. Simulating Binary Matrices:

Let $\mathbf{r} = (r_1, \ldots, r_m)$ and $\mathbf{s} = (s_1, \ldots, s_n)$ be integer sequences such that $\mathfrak{A}(\mathbf{r}, \mathbf{s})$ is not empty. For convenience, write $\mathfrak{A} = \mathfrak{A}(\mathbf{r}, \mathbf{s})$.

We will need notation for some other spaces of binary matrices. Let $\mathfrak{A}' = \cup \mathfrak{A}(\mathbf{r}', \mathbf{s}')$, where the union is taken over sequences $\mathbf{r}' = (r'_1, \ldots, r'_m)$ $\mathbf{s}' = (s'_1, \ldots, s'_n)$ such that

$$\begin{aligned} r'_i &= r_i - 1 \qquad & r'_k &= r_k, \quad k \neq i \\ s'_j &= s_j - 1 \qquad & s'_l &= s_l, \quad l \neq j \end{aligned}$$

for some indices i and j. Similarly, let $\mathfrak{A}'' = \cup\mathfrak{A}(\mathbf{r}'', \mathbf{s}'')$, where $\mathbf{r}'' = (r_1'', \ldots, r_m'')$, $\mathbf{s}'' = (s_1'', \ldots, s_n'')$, and

$$\begin{array}{lll} r'_{i_1} = r_{i_1} - 1 & r'_{i_2} = r_{i_2} - 1 & r'_k = r_k, \quad k \neq i_1, i_2 \\ s'_{j_1} = s_{j_1} - 1 & s'_{j_2} = s_{j_2} - 1 & s'_l = s_l, \quad l \neq j_1, j_2 \end{array}$$

for pairs of indices i_1, i_2 and j_1, j_2. Let $\mathcal{S} = \mathfrak{A} \cup \mathfrak{A}' \cup \mathfrak{A}''$.

Let $M \in \mathfrak{A}$. Define transitions for a Markov chain on $\mathfrak{A}$ as follows:

i. Select two entries m_{uv} and m_{rs} uniformly at random from the entries in M equal to 1.

ii. If $m_{us} = m_{rv} = 0$, interchange m_{uv} and m_{rs} with m_{us} and m_{rv}.

iii. Otherwise, do nothing.

Let P be a transition matrix corresponding to this transition scheme. Let $\pi(M) = |\mathfrak{A}|^{-1}$, $M \in \mathfrak{A}$. Then, it is not hard to show that π satisfies the detailed balance equations for P. If $\{X_n\}$ is a Markov chain on $\mathfrak{A}$ with these transitions then $\{X_n\}$ is reversible, with stationary measure π.

We wish to estimate the rate of convergence of the distribution of X_n to π. As in Section 3, we will construct a system of canonical paths in $\mathfrak{A}$. The construction will be done so that for any matrices J and F in $\mathfrak{A}$ and any edge $\{M, M'\}$ lying on the canonical path from J to F, we can map (J, F) uniquely to a matrix in $\mathcal{S}$.

Proposition 6. *There exists a set Γ of paths joining every pair of points in $\mathfrak{A}$ such that the number of paths containing a fixed edge is bounded above by $2\left(\binom{m-1}{2} + 1\right)|\mathcal{S}|$.*

Proof: Let $J, F \in \mathfrak{A}$ and suppose $J \oplus F = C$, where C is an elementary circuit. There is a standard algorithm for transforming J to F by interchanges. (See, for example, Brualdi[2], Section 3.) Let C have edges $\{x_1, y_1\}, \{y_1, x_2\}, \{x_2, y_2\}, \ldots, \{x_k, y_k\}, \{y_k, x_1\}$. Without loss of generality, suppose the matrices representing J and F have $J_{11} = J_{22} = \ldots = J_{kk} = 1$, $J_{12} = J_{23} = \ldots = J_{k-1,k} = J_{k1} = 0$, $F_{11} = F_{22} = \ldots = F_{kk} = 0$, $F_{12} = F_{23} = \ldots = F_{k-1,k} = F_{k1} = 1$, and $J_{ij} = F_{ij}$ elsewhere. Let p be the smallest integer such that $J_{p1} = 0$; $J_{k1} = 0$, so $p \leq k$. The first p interchanges will be $(p, p-1; 1, p), (p-1, p-2; 1, p-1), \ldots (2, 1; 1, 2)$.

$$\begin{pmatrix} 1 & 0 & & & & & \\ 1 & 1 & 0 & & & & \\ 1 & \ast & 1 & 0 & & & \\ 0 & \ast & \ast & 1 & 0 & & \\ 1 & \ast & \ast & \ast & 1 & 0 & \\ 1 & \ast & \ast & \ast & \ast & 1 & 0 \\ 0 & \ast & \ast & \ast & \ast & \ast & 1 \end{pmatrix} \qquad \begin{pmatrix} 0 & 1 & & & & & \\ 1 & 0 & 1 & & & & \\ 1 & \ast & 0 & 1 & & & \\ 0 & \ast & \ast & 0 & 1 & & \\ 1 & \ast & \ast & \ast & 0 & 1 & \\ 1 & \ast & \ast & \ast & \ast & 0 & 1 \\ 1 & \ast & \ast & \ast & \ast & \ast & 0 \end{pmatrix}$$

(a) *(b)*

$$\begin{pmatrix} 1 & 1 & & & & & \\ 0 & 1 & 1 & & & & \\ 0 & \ast & 1 & 1 & & & \\ 0 & \ast & \ast & 1 & 1 & & \\ 0 & \ast & \ast & \ast & 1 & 1 & \\ 0 & \ast & \ast & \ast & \ast & 1 & 1 \\ 1 & \ast & \ast & \ast & \ast & \ast & 1 \end{pmatrix} \qquad \begin{pmatrix} 0 & 1 & & & & & \\ 1 & 0 & 1 & & & & \\ 1 & \ast & 0 & 1 & & & \\ 1 & \ast & \ast & 0 & 0 & & \\ 1 & \ast & \ast & \ast & 1 & 0 & \\ 1 & \ast & \ast & \ast & \ast & 1 & 0 \\ 0 & \ast & \ast & \ast & \ast & \ast & 1 \end{pmatrix}$$

(c) *(d)*

Figure 1. The matrices *(a)* J, *(b)* F, *(c)* $J \oplus F$, and *(d)* J', where $m = n = 7$, $p = 4$

These p interchanges produce a matrix J' where $J'_{p+1,1} = J'_{p+2,p+2} = \ldots = J'_{kk} = 1$, $J'_{p+1,p+2} = \ldots = J'_{k-1,k} = J'_{k,1} = 0$, and $J'_{ij} = F_{ij}$ elsewhere. (See Figure 1 for typical examples of J, F, $J \oplus F$, and J'.) Repeating this process will eventually transform J to F. Note that this algorithm proceeds by unwinding a series of elementary circuits which are contained in C, with the possible exception of one edge. Call these circuits *subsidiary*.

It will be convenient to represent canonical paths somewhat differently. Associate each matrix $A \in \mathfrak{A}$ with the matrix $\tilde{A} = \mathrm{diag}(M, 1, 1)$. We can map the canonical path from J to F to a somewhat different path from $\tilde{J}$ to $\tilde{F}$ As before, let p be the smallest integer such that $J_{p1} = 0$. Let the first interchange in the canonical path from $\tilde{J}$ to $\tilde{F}$ be $(1, m+1; 1, n+1)$. If $p = 2$, let the second interchange be $(1, 2; n+1, 2)$; otherwise, let the second interchange be $(p, m+2; p, n+2)$. The next $p-1$ interchanges will be $(m+2, p-1; p, p-1), (m+2, p-2; p-1, p-2), \ldots, (m+2, 1; 2, 1), (1, m+2; 1, n+1)$; these correspond precisely to the interchanges $(p, p-$

$1; 1, p), (p-1, p-2; 1, p-1), \ldots, (2,1;1,2)$. Finally, make the interchange $(1, p; n+1, n+2)$. The unwinding will continue using the $(p, n+1)$ entry.

Let $\{M, M'\}$ be an edge in the canonical path from J to F. Without loss of generality, write the corresponding interchange as $(l, l-1; 1, l)$. We can translate this to an interchange on the modified canonical path in a standard fashion. Suppose $\{M, M'\}$ lies on a subsidiary cycle, with initial entry q and final entry p. Transform M and M' by the interchanges $(q, m+1; 1, n+1)$, $(l, m+2; l, n+2)$, $(l, p+1; 1, n+1)$ and $(q, m+1; 1, n+1)$, $(l-1, m+2; l-1, n+2)$, $(l-1, p+1; 1, n+1)$, respectively. This will transform M and M' into matrices M^* and $M^{*\prime}$ such that M^* is joined to $M^{*\prime}$ by the interchange $(l-1, m+2; l, l-1)$. Alternatively, suppose $\{M, M'\}$ does not lie on a subsidiary cycle. Then it is easy to see that $(l, l-1; 1, l)$ corresponds to the interchange $(l, l-1; n+1, l)$. To summarize, each edge $\{M, M'\}$ in the interchange graph can be transformed to a modified edge $\{M^*, M^{*\prime}\}$ by either one or three interchanges.

The first $p+1$ interchanges transform $\tilde{J}$ into a matrix $\tilde{J}'$, where $\tilde{J}'_{p+2,p+2} = \ldots = \tilde{J}'_{kk} = 1$, $\tilde{J}'_{p+1,p+2} = \tilde{J}'_{p+2,p+3} = \ldots = \tilde{J}'_{k-1,k} = \tilde{J}'_{k1} = 1$, and $\tilde{J}'_{ij} = \tilde{F}_{ij}$ for all other $1 \le i \le m$, $1 \le j \le n$. Again, we can repeat this process to transform $\tilde{J}$ into $\tilde{F}$ eventually.

Now, suppose $J \oplus F$ has connected components $G_1, \ldots, G_r$, and let G be one of these components. As in Section 3, specify a starting vertex for each G_i and order the Eulerian circuits starting from that vertex. By Lemma 4, each G_i has at least one Eulerian circuit in which entries from J and F alternate. Let γ be the first such circuit. Write γ as $\{x_1, y_1, x_2, y_2, \ldots, x_\nu, y_\nu, x_1\}$. Let $\rho = \min\{j : x_j = x_i, i < j\} \wedge \min\{j : y_j = y_i, i < j\}$, and let $j(\rho)$ be the unique $j < \rho$ such that $x_j = x_\rho$ or $y_j = y_\rho$. Then $\{x_{j(\rho)}, y_{j(\rho)}\}, \ldots, \{y_{\rho-1}, x_\rho\}$ or $\{y_{j(\rho)}, x_{j(\rho)+1}\}, \ldots, \{x_\rho, y_\rho\}$, as the case may be, forms an elementary circuit, which we denote C_1. Repeating this argument successively on $G \setminus C_1$, $G \setminus (C_1 \cup C_2)$ and so forth, we come to an ordered decomposition of G into elementary circuits $C_1, \ldots, C_k$.

Since γ is an alternating Eulerian circuit, each C_i is an alternating elementary circuit. We can pass from J to F by successively unwinding $G_1, \ldots, G_r$. In turn, each component G_j can be unwound by unwinding the elementary circuits $C_{j,1}, \ldots, C_{j,k_j}$

in order. So the unwinding algorithm for elementary circuits extends to an unwinding algorithm for Eulerian circuits, thence for the difference between elements in $\mathfrak{A}$.

To count canonical paths containing $\{M', M\}$, we will first encode modified paths containing $\{M^{*\prime}, M^*\}$ as a pair $(\rho, \sigma) \in \{+1, -1\} \times \mathcal{S}$. Let $\tilde{J} = \text{diag}(J, 1, 1)$, $\tilde{F} = \text{diag}(F, 1, 1)$, and let $S(\tilde{J}, \tilde{F})$ be the principal $m \times n$ submatrix of $\tilde{J} \oplus \tilde{F} \oplus (M^{*\prime} \vee M^*)$. The degree sequence of S will depend on the position of $\{M^{*\prime}, M^*\}$ in the unwinding. There are three possible cases:

i. $\{M^{*\prime}, M^*\}$ ends an elementary circuit.

ii. $\{M^{*\prime}, M^*\}$ lies inside an elementary circuit, but is not on a subsidiary circuit. Let x_i be the starting vertex of the elementary circuit, and let y_j be the current vertex being changed. Calculations similar to those in section 3 show that $\deg_S(x_i) = r_i - 1$, $\deg_S(y_j) = s_j + 1$. Furthermore, it is not hard to see that the first edge (i, i') of the current elementary circuit is in S.

iii. $\{M^{*\prime}, M^*\}$ lies on a subsidiary circuit, with starting edge $\{p, p'\}$ and ending edge $\{q, q'\}$. As before, we will have $\deg_S(x_i) = r_i - 1$, $\deg_S(y_j) = s_j + 1$. Also $\deg_S(x_p) = r_p + 1$, and $\deg_S(x_q) = r_q + 1$, and the edges $\{p, p'\}$, and $\{q, q'\}$ are in S.

With this in mind, define

$$\sigma(\tilde{J}, \tilde{F}) = \begin{cases} S(\tilde{J}, \tilde{F}) & \text{in case } i. \\ S(\tilde{J}, \tilde{F}) - e_{i,i'} & \text{in case } ii. \\ S(\tilde{J}, \tilde{F}) - e_{i,i'} - e_{p,p'} - e_{q,q'} & \text{in case } iii. \end{cases}.$$

and

$$\rho(\tilde{J}, \tilde{F}) = \begin{cases} +1 & \text{in cases } i. \text{ and } ii. \\ +1 & \text{in case } iii., \text{ if } (p-q)(p'-q') > 0 \\ -1 & \text{in case } iii., \text{ if } (p-q)(p'-q') < 0. \end{cases}$$

Here, $e_{i,i'}$, $e_{p,p'}$, and $e_{q,q'}$ are the edges joining $\{i, i'\}$, $\{p, p'\}$, and $\{q, q'\}$, respectively.

Examining the definition will show that $\sigma(\tilde{J}, \tilde{F}) \in \mathfrak{A}$ in case *i.*, $\sigma(\tilde{J}, \tilde{F}) \in \mathfrak{A}'$ in case *ii.*, and $\sigma(\tilde{J}, \tilde{F}) \in \mathfrak{A}''$ in case *iii.*

We claim that we can determine J and F from (ρ, σ) and $\{M^*M^{*\prime}\}$. To see this, first observe that we can reconstruct $S(\tilde{J}, \tilde{F})$ from (ρ, σ). In cases *i.* and *ii.*, this is identical to the argument in Section 3. In case *iii.*, we have to identify the edges $e_{i,i'}$, $e_{p,p'}$, and $e_{q,q'}$ and restore them to σ to obtain S..

Since there are precisely two rows in σ with diminished row sums, one of which corresponds to $M^* \oplus M^{*\prime}$, and since $M^*[n+1, i'] = 1$, reconstructing $e_{i,i'}$ is automatic. To reconstruct $e_{p,p'}$ and $e_{q,q'}$, note that $M^*[p, n+1] = M^*[q, n+2] = 1$, $s'_{p'} = s_{p'} - 1$, and $s'_{q'} = s_{q'} - 1$. This leaves two possible pairs of edges, which are distinguished by the value of ρ.

Knowing $S(\tilde{J}, \tilde{F})$, we can reconstruct J and F by an argument similar to that in Section 3. Let $J \oplus F$ have connected components $G_1, \ldots, G_r$. There is a unique component G_κ containing the edges $\{u, v\}$ and $\{v, u'\}$. For $j \neq \kappa$, let γ_j be the first Eulerian path on G_j such that edges in S and $M^* \vee M^{*\prime}$ alternate. For $1 \leq j < \kappa$, odd parity edges are in J and even parity edges are in F; for $\kappa < j \leq r$, the parity of edges is reversed. Let γ_κ be the first Eulerian path on G_κ such that its elementary circuit decomposition $E_1, \ldots, E_\rho$ gives even parity to edges in S preceding $\{u, v\}$ and odd parity to edges in S following $\{v, u'\}$. Odd parity edges preceding $\{u, v\}$ and even parity edges following $\{v, u'\}$ are in J; Even parity edges preceding $\{u, v\}$ and odd parity edges following $\{v, u'\}$ are in F. Thus, J and F can be reconstructed from $M^* \vee M^{*\prime}$ by adding and deleting appropriate edges.

Since $(J, F) \rightarrow \sigma(\tilde{J}, \tilde{F})$ is invertible, it follows that the mapping is one–to–one. Each encoding $\sigma(\tilde{J}, \tilde{F})$ is in $\mathcal{S}$. Thus, the number of canonical paths containing $\{M^{*\prime}, M^*\}$ is at most $|\mathcal{S}|$.

It remains to compute the number of modified transitions $\{M^{*\prime}, M^*\}$ corresponding to each possible transition $\{M', M\}$. Depending on its position in the the elementary circuit E, each transition $\{M', M\}$ can be transformed to a modified transition $\{M^{*\prime}, M^*\}$ by either one or three interchanges. If one interchange is required, then the interchange affects one of the two vertices in $M \backslash M'$; this gives two possible pairs $\{M^{*\prime}, M^*\}$. If three interchanges are required, then $\{M', M\}$ lies on a subsidiary cycle. Thus, we need to choose the beginning and the end of the subsidiary cycle, by choosing any two ones in a column modified by $\{M', M\}$. This can be done in at most $2\binom{m-1}{2}$ possible ways. Thus there are at most $2\binom{m-1}{2}+2$ pairs $\{M^{*\prime}, M^*\}$ corresponding to each pair $\{M', M\}$. The total number of canonical paths crossing $\{M', M\}$ is then at most

$$2\left(\binom{m-1}{2}+1\right)|S| \quad \blacksquare$$

As before, the estimate of the number of canonical paths gives an estimate of the subdominant eigenvalue of the transition matrix of $\{X_n\}$.

Proposition 7.

$$\beta_1 \leq 1 - \frac{1}{8} \cdot \left(2\binom{N}{2}\left(\binom{m-1}{2}+1\right) \cdot \frac{|S|}{|\mathfrak{A}|}\right)^{-2}$$

Proof: Again, we have $\eta = \max_e Q(e)^{-1} \sum_{\gamma_{xy} \ni e} \pi(x)\pi(y)$. Using our bound on the number of canonical paths,

$$\begin{aligned}
\eta &\leq |\mathcal{E}| \cdot 2\left(\binom{m-1}{2}+1\right) \cdot |S| \cdot \frac{1}{|\mathfrak{A}|^2} \\
&= 2\left(\binom{m-1}{2}+1\right) \cdot \frac{|\mathcal{E}|}{|\mathfrak{A}|} \cdot \frac{|S|}{|\mathfrak{A}|} \\
&\leq 2\binom{N}{2} \cdot \left(\binom{m-1}{2}+1\right) \cdot \frac{|S|}{|\mathfrak{A}|}
\end{aligned}$$

The proposition now follows from Theorem 2. $\blacksquare$

Proposition 8. *Let $\mathfrak{A} = \mathfrak{A}(\mathbf{r}, \mathbf{s})$. Then a sufficient condition for $|S|/|\mathfrak{A}|$ to be polynomially bounded is that $N > 2(r_{max}-1)(s_{max}-1)+1$.*

Proof: Let $(r'_1, \ldots, r'_m)$ and $(s'_1, \ldots, s'_n)$ be the row and column sums for a matrix in $\mathfrak{A}'$. Then $(r'_{max}-1)(s'_{max}-1) \leq (r_{max}-1)(s_{max}-1)$. Suppose $N > 2(r_{max}-1)(s_{max}-1)+1$. Then $N-1 > 2(r_{max}-1)(s_{max}-1) \geq 2(r'_{max}-1)(s'_{max}-1)$, so $\mathfrak{A}((r'_1, \ldots, r'_m); (s'_1, \ldots, s'_n))$ is itself a p-stable set. As the number of possible sequences $(r'_1, \ldots, r'_m)$ and $(s'_1, \ldots, s'_n)$ is a polynomial in m and n, it follows that the $|S|/|\mathfrak{A}|$ is polynomially bounded. $\blacksquare$

Our estimate of β_1 gives a bound on the average error committed by using sample averages of our Markov chain to approximate integrals. We state our bound for a general chain.

Let $\{X_n\}$ be a Markov chain on a finite state space, with stationary distribution π. Let f be a function and let $\mu_f = \sum f(x)\pi_x$, $\sigma_f^2 = \sum(f(x) - \mu_f)^2\pi_x$. For $m, n > 0$, let $A_{m,n} = n^{-1}\sum_m^{m+n} f(X_i)$. If E_x denotes expectation for the chain with $X_0 = x$, then the following estimate is routine:

Proposition 9.

$$E_x(A_{m,n} - \mu_f)^2 \leq \frac{2}{n(1-\beta_1)}\left(1 + \pi_*^{-1}\beta_1^m\right)\left(1 + \frac{1}{n(1-\beta_1)}\beta_1^n\right)\sigma_f^2 \qquad (13)$$

where $\pi_* = \min_x \pi(x)$.

Proof: For $m \sim \text{Poisson}(N)$, this estimate is given in Aldous[1] Proposition 4.2, with β_1^N in place of β_1^m and some differences in notation. For fixed m, it suffices to follow the argument given in Aldous to his expression (4.9), and then to observe that for any fixed $m \geq 0$ and any λ, $\lambda^m = (1 + (\lambda - 1))^m \leq \exp(m(\lambda - 1))$. ∎

Let $\{X_n\}$ be the Markov chain on $\mathfrak{A}$, with transition matrix P, and suppose we wish to estimate μ_f for some function f; here, $\pi(x) \equiv |\mathfrak{A}|^{-1}$. To estimate μ_f with MSE smaller than ϵ, we can take $m \geq \log M/\log\beta_1$, giving $1 + |\mathfrak{A}|\beta_1^m \leq 2$. Then take $n \geq 8\sigma_f^2/\epsilon(1 - \beta_1)$ to give $E_x(A_{m,n} - \mu_f)^2 < \epsilon$.

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